A short tutorial on Green's functions

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Abstract

This publication gives a short introduction to Green's function as used in theoretical solid state physics (and also in quantum field theories). Second quantization is presented and the perturbation theory based on Green's functions for zero temperature is derived. Feynman diagrams are explained.

Contents

1 Introduction

> *"... It might be noted, for the benefit of those interested in exact solutions, that there is an alternative formulation of the many-body problem, i.e., how many bodies are required before we have a problem? G.E. Brown points out, that this can be answered by a look at history. In eighteenth-century Newtonian mechanics, the three-body problem was insoluble. With the birth of general relativity around 1910 and quantum electrodynamics in 1930, the two- and one-body problems became insoluble. And within modern quantum field theory, the problem of zero bodies (vacuum) is insoluble. So, if we are out after exact solutions, no bodies is already too many!"*
> (in: R.D. Mattuck, A Guide to Feynman Diagrams in the Many-Body Problem)[1]

Only a few problems in quantum mechanics can be solved exactly. Therefore, one is dependent upon approximation schemes. One of these is perturbation theory. In perturbation theory, the Hamiltonian H of the system under investigation is split into a "trivial," that is, exactly solvable part H_0, and a perturbation V and written as

$$H = H_0 + V \ .$$

Perturbation theory then uses the knowledge of the solution to H_0 (i.e., of its eigenfunctions $|n\rangle_0$ and eigenvalues E_n^0) together with the perturbation V to give an approximation to the solution of the full Hamiltonian H. In its simplest form, for the case of a one-particle problem with a discrete non-degenerate spectrum, the eigenvalues E_n of H are approximated by $E_n \approx E_n^0 + {}_0\langle n|V|n\rangle_0$ to first order in V.

It is clear that in the case of a many-particle system, the things are getting much more complicated, but surprisingly, a very nice and physically transparent perturbation theory can be given. This perturbation theory is based on Green's functions which characterize a quasi-particle in the sense

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[1] Despite of having taking this citation out of the many-particle book of Mattuck [1], most of the material here resembles quite close the introduction presented in the book of Mahan [2] with traces from the book of Abrikosov, Gorkov, and Dzyaloshinski [3]. Also very instructive is the book of Landau and Lifshitz [4]. For those who like to give an eye to applications in physics, the book of Schrieffer [5] is great.

of Landau's Fermi liquid theory (see [4]. Landau, however, did not make use of Green's functions in his theory). We are going to present this theory in the appendix at hand.

2 Second quantization

The first forms of quantum mechanics given by Schrödinger's wave equation and Heisenberg's matrices though originally developed for the description of systems with single particles, can also be applied to a system with a fixed number N of identical particles. Nevertheless this is very cumbersome, mainly because of the Pauli principle forcing the wave functions to be antisymmetric (fermions) or symmetric (bosons) when exchanging two particles. Antisymmetrizing wave functions (usually done by using a Slater determinants) is rather complicated and error-prone. Therefore, a different representation for quantum mechanics, the *second quantization*, has been developed to remove the problems just mentioned. Indeed, second quantization removes the problem of antisymmetrizing (or symmetrizing) wave functions—the formalism of second quantization automatically takes care of that. Additionally, it allows for the treatment of systems with a varying number of particles, such as phonon or photon systems, or for the treatment of the superconducting state as formulated in the BCS-theory.

Quantum mechanics, in its original formulation, deals with operators acting on wave functions. This is also the case in the formulation provided by second quantization. But the operators used in second quantization are rather different from those in the original formulation which we call the *first quantization*. In first quantization we have learned how to describe a given physical system by means of the Hamilton operator. The description of the physical system in second quantization is based as well on a Hamilton operator, but its form is completely different from that of the former. One of our goals here is to show how to construct the Hamiltonian used to describe a given physical system in second quantization when the corresponding Hamiltonian for first quantization is given.

Let us first summarize the treatment of a system of a fixed number N of identical particles in first quantization. If one of the particles is described by the Hamiltonian

$$h_0(\boldsymbol{p}, \boldsymbol{r}) = \frac{1}{2m}\boldsymbol{p}^2 + U(\boldsymbol{r}) \ ,$$

the collection of N identical and not interacting particles is represented by the N-particle Hamiltonian

$$H_0 = \sum_{i=1}^{N} h_0(\boldsymbol{p}_i, \boldsymbol{r}_i) \tag{1}$$

where the operators $\boldsymbol{p}_i$ and $\boldsymbol{r}_i$ are acting on the particle i. The wave functions of the N-particle system are

$$\psi(\boldsymbol{r}_1 \ldots, \boldsymbol{r}_N)$$

which can be written as a linear combination of the functions

$$\psi_{\boldsymbol{k}_1}(\boldsymbol{r}_1) \cdot \ldots \cdot \psi_{\boldsymbol{k}_N}(\boldsymbol{r}_N) \ ,$$

that is, products of single particle wave functions $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ which are usually chosen to be eigenfunctions of the Hamiltonian h_0, and therefore given by

$$h_0 \psi_{\boldsymbol{k}}(\boldsymbol{r}) = \epsilon_{\boldsymbol{k}} \psi_{\boldsymbol{k}}(\boldsymbol{r}) \ ,$$

where $\boldsymbol{k}$ is a quantum number denoting a stationary state of the single-particle Hamiltonian h_0. In a translationally invariant system or a crystal, this may be the momentum or quasimomentum, respectively, together with a spin index if the particles under discussion carry such property. Note that these N-particle wave functions have to be antisymmetrized (we focus on fermion systems; for bosonic systems, the wave function has to be symmetrized), and therefore, all the single particle states $\boldsymbol{k}_i$ have to be different. Otherwise the wave function vanishes, expressing the fact that a single-particle state can be occupied only once in fermionic systems.

A translationally invariant two-particle interaction as for instance the Coulomb interaction is represented in the N-particle system by the Hamiltonian

$$H_I = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

summing over all combinations of two particles. The factor 1/2 compensates for a double-counting in the sum over i and j.

2.1 Creation and destruction operators

In second quantization, new operators are introduced. These are the *creation* and *destruction* operators. Given a state $|\rangle$, the creation operator c^+_λ adds a particle in the single-particle state ψ_λ to $|\rangle$. If $|\rangle$ is an N-particle state, then $c^+_\lambda|\rangle$ is an $(N+1)$-particle state. If the state $|\rangle$ already contains a particle in state λ, the expression $c^+_\lambda|\rangle$ vanishes. The destruction[2] operator c_λ works in a similar way. It removes a particle in the single-particle state λ from the (many-body) state $|\rangle$, and destroys the entire many-body state, if such particle was not there. As the notation suggests, the creation and destruction operators are mutually hermitian conjugate.

For bosons, creation and destruction operators b^+_λ and b_λ are also defined. They work similarly to their fermion-colleagues, but allow for a multiple-occupancy of the single-particle states. That is, the creation operator b^+_λ never annihilates a state $|\rangle$, whether it already contained particles in the single-particle state λ or not.

These properties of the fermionic and bosonic creation and destruction operators are guaranteed by anticommutation and commutation rules, respectively. For fermions, the anticommutators

$$\begin{aligned} \{c_\lambda, c_\mu\} &= \{c^+_\lambda, c^+_\mu\} = 0 \\ \{c_\lambda, c^+_\mu\} &= \{c^+_\mu, c_\lambda\} = \delta_{\lambda\mu} \end{aligned} \tag{2}$$

guarantee antisymmetry, because $c_\lambda c_\mu = -c_\mu c_\lambda$, and prevent from double-occupancy because for $\mu = \lambda$, we have $c_\lambda c_\lambda = -c_\lambda c_\lambda = 0$. The second relation (2) taken for $\mu = \lambda$ determines the eigenvalues of the creation and destruction operators. Applied to a state $|\rangle$, it yields $c_\lambda c^+_\lambda|\rangle + c^+_\lambda c_\lambda|\rangle = |\rangle$. If the single-particle state λ is occupied in $|\rangle$, the first term in the sum will vanish whereas the second one reproduces $|\rangle$ with a factor of one. If the state is unoccupied, the first term yields a factor of one, while the second vanishes.

For the bosonic operators, which have to express the fact that many-particle states of a system composed of identical bosonic particles are symmetric upon exchange of two particles, the commutation relations

$$\begin{aligned} [b_\lambda, b_\mu] &= [b^+_\lambda, b^+_\mu] = 0 \\ [b_\lambda, b^+_\mu] &= -[b^+_\mu, b_\lambda] = \delta_{\lambda\mu} \end{aligned} \tag{3}$$

hold and describe the fact that single-particle boson states can be occupied multiply.

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[2] We use the terms "destruction operator" and "annihilation operator" interchangeably.

Note that because of their non-hermiticity, the creation and destruction operators are not observable. The importance of these operators lies in the fact that all other operators can be expressed as linear combinations of products of creation and destruction operators. An example are the particle number operator N, and the Hamiltonian H_0, which are given by

$$N = \sum_{\boldsymbol{k}} n_{\boldsymbol{k}} = \sum_{\boldsymbol{k}} c^+_{\boldsymbol{k}} c_{\boldsymbol{k}} \qquad \text{and} \qquad H_0 = \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} c^+_{\boldsymbol{k}} c_{\boldsymbol{k}} \ . \tag{4}$$

where $n_{\boldsymbol{k}}$ is the number operator counting the number of particles in the single-particle state $\boldsymbol{k}$, and $\epsilon_{\boldsymbol{k}}$ is the single-particle dispersion relation. States which are eigenstates to the particle number operator N contain a fixed number of particles.

We introduce next the rules for determining the form that an operator given in first quantization assumes the second quantization. One-particle operators of the form $O^{(1)} = \sum_i O^{(1)}(\boldsymbol{p}_i, \boldsymbol{r}_i)$ are expressed in second quantization as

$$\begin{aligned} O &= \sum_{\alpha\beta} c^+_\alpha O^{(1)}_{\alpha\beta} c_\beta \qquad \text{with} \\ O^{(1)}_{\alpha\beta} &= \langle\alpha|O^{(1)}|\beta\rangle = \int d^3r\, \psi^*_\alpha(\boldsymbol{r}) O^{(1)}(\boldsymbol{p}, \boldsymbol{r}) \psi_\beta(r) \end{aligned} \tag{5}$$

For a two-particle operator

$$O^{(2)} = \sum_{i \neq j} O^{(2)}(\boldsymbol{p}_i, \boldsymbol{r}_i; \boldsymbol{p}_j, \boldsymbol{r}_j)$$

its corresponding second quantized operator O becomes

$$\begin{aligned} O &= \sum_{\alpha\beta\gamma\delta} c^+_\alpha c^+_\beta O^{(2)}_{\alpha\beta\gamma\delta} c_\gamma c_\delta \qquad \text{with} \\ O^{(2)}_{\alpha\beta\gamma\delta} &= \langle\alpha\beta|O^{(2)}|\gamma\delta\rangle \\ &= \int d^3r\, d^3r'\, \psi^*_\alpha(\boldsymbol{r}) \psi^*_\beta(\boldsymbol{r}') O^{(2)}(\boldsymbol{p}, \boldsymbol{r}; \boldsymbol{p}', \boldsymbol{r}') \psi_\gamma(\boldsymbol{r}') \psi_\delta(\boldsymbol{r}) \end{aligned} \tag{6}$$

The application of these rules to H_0 is easy. Suppose the external potential $U(r)$ vanishes. Then plane waves are eigenstates of the single-particle Hamiltonian h_0 (for simplicity we disregard the spin), and because of the relationship

$$\int d^3r\, e^{-i\boldsymbol{k}_\alpha \boldsymbol{r}} \frac{\boldsymbol{p}^2}{2m} e^{-i\boldsymbol{k}_\beta \boldsymbol{r}} = \frac{\boldsymbol{k}^2_\alpha}{2m} \delta_{\alpha\beta} \ ,$$

the second quantized Hamiltonian for the non-interacting system is given by the equation

$$H_0 = \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} c^+_{\boldsymbol{k}} c_{\boldsymbol{k}} \qquad \text{with} \qquad \epsilon_{\boldsymbol{k}} = \frac{\boldsymbol{k}^2}{2m} \ . \tag{7}$$

The translation of a two-particle operator like the Coulomb interaction to the second quantized form is more delicate. According to (6), for a system with continuous translational symmetry we have to evaluate the integral

$$V_{\boldsymbol{k}_\alpha \boldsymbol{k}_\beta \boldsymbol{k}_\gamma \boldsymbol{k}_\delta} \int d^3r \, d^3r' \, e^{i(\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta)\boldsymbol{r}} e^{i(\boldsymbol{k}_\beta - \boldsymbol{k}_\gamma)\boldsymbol{r}'} \frac{4\pi e^2}{|\boldsymbol{r} - \boldsymbol{r}'|}$$

Using $\boldsymbol{k}_\alpha = \boldsymbol{k} + \boldsymbol{q}$, $\boldsymbol{k}_\beta = \boldsymbol{k}' - (\boldsymbol{q} + \vec{\delta})$, $\boldsymbol{k}_\gamma = \boldsymbol{k}'$, and $\boldsymbol{k}_\delta = \boldsymbol{k}$, the exponentials can be written as $\exp(i\boldsymbol{q}(\boldsymbol{r} - \boldsymbol{r}')) \cdot \exp(-i\vec{\delta}\boldsymbol{r}')$. The fact that the Coulomb interaction just depends on the difference $\boldsymbol{r} - \boldsymbol{r}'$, and not on $\boldsymbol{r}$ and $\boldsymbol{r}'$ individually, implies that $\vec{\delta} = 0$, otherwise the integral would vanish. We are then left with the expression

$$V_{\boldsymbol{k}+\boldsymbol{q}, \boldsymbol{k}' - (\boldsymbol{q}+\vec{\delta}), \boldsymbol{k}', \boldsymbol{k}} = \delta_{\vec{\delta},0} \int d^3r \, d^3r' \, \frac{e^{-i\boldsymbol{q}(\boldsymbol{r}-\boldsymbol{r}')}}{|\boldsymbol{r} - \boldsymbol{r}'|} = \Omega \cdot \frac{4\pi e^2}{q^2} \delta_{\vec{\delta},0}$$

where Ω is the integration volume. This matrix element only depends on the differences $\boldsymbol{k}_\alpha - \boldsymbol{k}_\delta$ and $\boldsymbol{k}_\beta - \boldsymbol{k}_\gamma$ of the momenta of the scattered and incoming electrons, respectively. This is a consequence of the continuous translational symmetry of the system. The fact that the interaction depends only on the coordinates through $|\boldsymbol{r} - \boldsymbol{r}'|$ implies that in the scattering process the two interacting electrons cannot exchange momentum nor angular momentum with the rest of the system (this is only valid for free electrons. In a crystal, the pseudopotential breaks the continuous translational symmetry as well as the rotational symmetry of the Hamiltonian). The scattering process conserves momentum. Putting the matrix element under discussion into the expression for the two-particle operator in second quantization leaves us with the expression

$$V = \frac{1}{2} \sum_{\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}} \frac{4\pi e^2}{q^2} c^+_{\boldsymbol{k}+\boldsymbol{q}} c^+_{\boldsymbol{k}'-\boldsymbol{q}} c_{\boldsymbol{k}'} c_{\boldsymbol{k}} \tag{8}$$

which can be represented in an obvious way by the diagram in Fig. 1. Two electrons with momenta $\boldsymbol{k}$ and $\boldsymbol{k}'$ are propagating. Then they interact and continue propagating with momenta $\boldsymbol{k} + \boldsymbol{q}$ and $\boldsymbol{k}' - \boldsymbol{q}$. The total momentum is conserved, the label $\boldsymbol{q}$ on the dashed line denotes the momentum transfer.

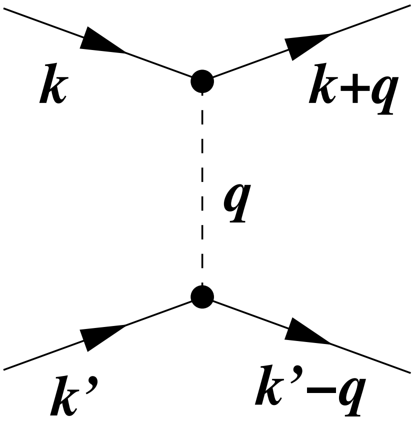

Figure 1: The Coulomb interaction.

2.2 Normalizations and Fourier transforms

A final word on the normalization of wave functions and, related to that, the use of Fourier transformations. The Fermion field operators are defined by $\Psi(\boldsymbol{r}) = \sum_\lambda a_\lambda \psi_\lambda(\boldsymbol{r})$ using the single particle wave functions $\psi_\lambda(\boldsymbol{r})$. We work in a box of volume V, therefore the normalization condition for the wave functions is $\int_V d^3r\, \psi_\lambda(\boldsymbol{r})\psi_{\lambda'}(\boldsymbol{r}) = \delta_{\lambda\lambda'}$. In the case of free particles, the wave functions are plane waves $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = V^{-1/2} \exp i\boldsymbol{kr}$.

The Fourier transformation for functions of time is given by the expressions

$$f(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} f(t) \qquad \text{and} \qquad f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t} f(\omega)$$

where the frequency ω is a continuous variable. For functions of space, the Fourier transform is given by

$$f_{\boldsymbol{k}} = \int_V d^3r\, e^{-i\boldsymbol{kr}} f(\boldsymbol{r}) \qquad \text{and} \qquad f(\boldsymbol{r}) = \frac{1}{V} \sum_{\boldsymbol{k}} e^{i\boldsymbol{kr}} f_{\boldsymbol{k}}$$

whereas the variable $\boldsymbol{k}$ is discrete. The adjacent values of $\boldsymbol{k}$ have a distance of $2\pi/L$, where $V = L^3$. When having to perform k-space summations, we can convert them to integrals. This is possible for large V, and done by substituting

$$\frac{1}{V}\sum_{\boldsymbol{k}} \to \int \frac{d^3k}{(2\pi)^3} \qquad \text{and} \qquad \delta_{\boldsymbol{k}\boldsymbol{k}'} \to \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}-\boldsymbol{k}') \ .$$

When manipulating expressions, we normally use the k-space summations and switch to integrals only if a k-space sum has to be calculated explicitly.

3 The zero-temperature Green's function

In perturbation theory, the many-body Hamiltonian H is split into a "simple" part H_0 (which is solvable exactly, that is, whose eigenfunctions and -energies are known), and a nontrivial part V, the particle-particle interaction treated as a *perturbation*. We denote the known ground state of the Hamiltonian H_0 by $|0\rangle$, and the ground state of the complete Hamiltonian H by $|\mathrm{GS}\rangle$. The latter is often referred to as the *exact* ground state to distinguish it from the former. Furthermore, the Hamiltonian H_0 is assumed to describe a collection of systems of identical particles as in (1), such that single-particle excitations are defined. Let us denote the wave functions describing these single-particle excitations by ψ_λ.

The first definition of the Green's function is given in the Heisenberg representation, in which the operators are time-dependent and the wave functions are not (see Tab. 1). This allows for a very clear physical interpretation of the Green's function.

The *zero-temperature Green's function* G for a system of electrons is given by the ground-state expectation value

$$G(\lambda, t-t') = -i\langle \mathrm{GS}|T\{c_{H,\lambda}(t)c^+_{H,\lambda}(t')\}|\mathrm{GS}\rangle \ . \tag{9}$$

In this definition, the Heisenberg operators[3] $c^+_{H,\lambda}(t)$ and $c_{H,\lambda}(t')$ create and destroy, respectively, an electron in the single-particle state ψ_λ, at the time t and t', respectively. The state ψ_λ is an eigenstate of the *unperturbed* Hamiltonian H_0 for the case when the system contains exactly *one* particle. In

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[3] We will use the Schrödinger-, Heisenberg-, and interaction-representation in this appendix. Operators or wave functions in the Schrödinger representation either will carry an index "S" or just no time-argument. The Heisenberg-representation is denoted by an index "H". In the interaction-representation, operators and wave functions just carry a time-argument.

Schrödinger rep.	Heisenberg rep.	interaction rep.
O_S $\psi_S(t) = e^{-iHt}\psi_S(0)$	$O_H(t) = e^{iHt}O_S e^{-iHt}$ $\psi_H = \psi_S(0)$	$O(t) = e^{iH_0t}O_S e^{-iH_0t}$ $\psi(t) = e^{iH_0t}\psi_S(t)$

Table 1: Definition of the representations under use.

the Heisenberg representation (see Tab. 1), the time-dependence of the c-operators is given by $c^+_{H,\lambda}(t) = \exp(iHt)c^+_{H,\lambda}(0)\exp(-iHt)$. The "operator" T is the time-ordering operator. Given two or more time-dependent operators, it orders these in such a way that the operators with later times are left ("the future is left"), and, additionally puts a minus sign for each interchange of two fermionic operators (i.e. anticommuting operators). The interchange of bosonic operators does not alter the sign. For the special case of two fermionic operators $A(t)$ and $B(t')$, this means

$$T\{A(t)B(t')\} = \begin{cases} A(t)B(t') & \text{for } t - t' > 0 \\ -B(t')A(t) & \text{for } t - t' < 0 \end{cases}$$

and leaves undetermined intentionally the case $t = t'$.

The *physical interpretation* of the Green's function (9) for the case $t > t'$ is as follows. At the time t', an electron in the single-particle state ψ_λ is added to the *exact* ground state $|\mathrm{GS}\rangle$. This electron then propagates in the system and interacts with other electrons as a consequence of not being in an eigenstate of the full Hamiltonian H. At a later time t, the electron is removed from the system. The quantity $G(\lambda, t - t')$ then describes the *amplitude* at the time of this removal. In the special case $V = 0$ of no present perturbation, the electron will stay in the state ψ_λ and the *magnitude* of $G(\lambda, t - t')$ will be one for all values of $t - t' > 0$.

4 Interaction representation and S-matrix

Although the definition given in (9) is physically rather clear, it poses some problems. First of all, the exact ground state $|\mathrm{GS}\rangle$ needed to evaluate (9) is not known: its determination is *the* essential problem of many-body theory. Second, there is no clear separation of the implications of the free part H_0 and the interaction part V of the Hamiltonian H on the Green's function.

This makes our goal of developing a perturbation theory for the determination of G unnecessarily difficult. These deficiencies will be remedied by restating (9) in the *interaction representation* (see Tab. 1) and introducing the S-matrix. The interaction representation makes the operators as well as the wave functions time-dependent. The trivial time-dependence generated by H_0 is put into the operators, and the nontrivial part, corresponding to V, is put into the wave functions by writing

$$\begin{aligned} O(t) &= e^{iH_0t} O_S e^{-iH_0t} \\ \psi(t) &= e^{iH_0t}\psi_S(t) = e^{iH_0t}e^{-iHt}\psi_S(0) = U(t)\psi_S(0) \ , \end{aligned}$$

where the unitary matrix $U(t) = e^{iH_0t}e^{-iHt}$ has been introduced. For vanishing perturbation $V = 0$, this matrix becomes the unit matrix, and therefore the interaction representation reverts to the Heisenberg representation. The S-matrix $S(t,t')$ can be defined by means of the U-matrix,

$$\psi(t) = S(t,t')\psi(t') = U(t)U^+(t')\psi(t') \ , \quad S(t,t') \equiv U(t)U^+(t') \tag{10}$$

it "takes ψ from t' to t." The S-matrix contains the time-evolution of the wave functions in the interaction representation. The properties of the S-matrix are the following:

1. $S(t,t') \equiv 1 \quad \text{if } V = 0$
2. $S(t,t) = 1$
3. $S(t,t')S(t',t'') = S(t,t'')$ (transitivity)
4. $S^+(t,t') = S(t',t)$ (time reversal).

The most important of these properties is the third one, it allows for the connection of two subsequent time-evolutions.

Just by calculating the time-derivative of the definition of the U-matrix, we can give the differential equation

$$\frac{d}{dt}U(t) = -iV(t)U(t) \tag{11}$$

which together with the condition $U(0) = 1$ can be used to determine $U(t)$ and, therefore, by (10) the S-matrix $S(t,t')$. The solution for $U(t)$ is given by integrating (11) once and iterating this process. This yields the series

$$U(t) = 1 - i\int_0^t dt_1\, V(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2\, V(t_1)V(t_2) + \cdots \tag{12}$$

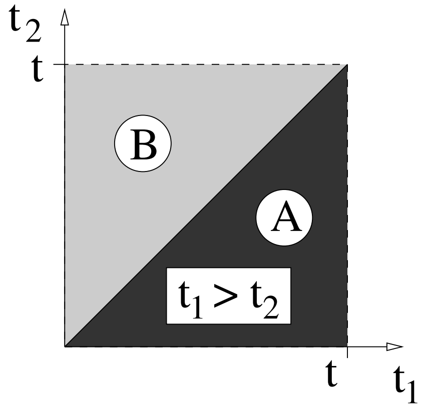

Figure 2: The integration volume for the correction to the S-matrix in second order perturbation theory.

which is an exact solution to (11). However, (12) is rather inconvenient because of the complicated integration limits, which, for the case of the term of second order in V are given by region A in Fig. 2. Exchanging t_1 and t_2 in the term of second order in V changes the integration region from region A to region B, but leaves the integral (12) unchanged. In both cases A and B, the two operators $V(t)$ in the integral are ordered in such a way that the operator acting at the later time is to the left. Therefore, the integral under consideration is equivalent to

$$\frac{(-i)^2}{2}\int_0^t dt_1 \int_0^t dt_2\, T\{V(t_1)V(t_2)\}\ ,$$

where the integration region is now a square. Arguing along the same lines for the other terms in the series (12), it can be shown that this series can be written in the form

$$U(t) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!}\int_0^t dt_1 \cdots \int_0^t dt_n\, T\{V(t_1)\cdots V(t_n)\}\ . \qquad (13)$$

If we use the definition of the exponential function and the convention that the time-ordering operator T operating on the exponential function is equivalent to operating on every term in the corresponding series expansion individually, the S-matrix (10) is given by the expression

$$\begin{aligned} S(t,t') &= 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} dt_1 \cdots \int_{t'}^{t} dt_n \, T\{V(t_1)\cdots V(t_n)\} \\ &= T \exp\left(-i \int_{t'}^{t} dt_0 \, V(t_0)\right) \end{aligned} \tag{14}$$

with the perturbation Hamiltonian V in the *interaction representation*.

By just introducing the interaction representation, our main problem that the exact ground state $|\mathrm{GS}\rangle$ is unknown, remains unsolved. But the S-matrix is the key to solve it. Gell-Mann and Low [6] have proven a theorem which states that the exact ground state $|\mathrm{GS}\rangle$ (which is time-independent in the Heisenberg representation) is given by

$$|\mathrm{GS}\rangle = S(0,-\infty)|0\rangle \ .$$

The exact ground state can thus be generated by applying the evolution generated by the S-matrix from $t = -\infty$ till $t = 0$ to the known ground state $|0\rangle$ of the unperturbed part of the Hamiltonian H_0.

Because of time reversal symmetry, it is clear that by applying the operator $S(\infty, 0)$ to the exact ground state $|\mathrm{GS}\rangle$, we will recover the ground state $|0\rangle$ of H_0 up to a phase.[4] That is,

$$S(\infty,0)|\mathrm{GS}\rangle = e^{i\varphi}|0\rangle \qquad \text{or} \qquad \langle 0|S(\infty,-\infty)|0\rangle = e^{i\varphi} \ ,$$

which is a very important relation allowing us to write the bra-vector $\langle\mathrm{GS}|$ as

$$\langle\mathrm{GS}| = \langle 0|S(-\infty,0) = \frac{\langle 0|S(\infty,0)}{\langle 0|S(\infty,-\infty)|0\rangle} \ .$$

We apply the results derived in the discussion above and especially the relation $c_{H,\lambda}(t) = S(0,t)c_\lambda(t)S(t,0)$ to the Green's function (9). This yields

$$\begin{aligned} &\langle\mathrm{GS}|c_{H,\lambda}(t)c^{+}_{H,\lambda}(t')|\mathrm{GS}\rangle \\ &\qquad = \frac{\langle 0|S(\infty,t)c_\lambda(t)S(t,t')c^{+}_\lambda(t')S(t',-\infty)|0\rangle}{\langle 0|S(\infty,-\infty)|0\rangle} \end{aligned} \tag{15}$$

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[4] We suppose that the ground state is a non-degenerate state. This is not the case in the strict sense for isotropic systems with a magnetic low-temperature phase or for gauge invariant systems with a superconducting low-temperature phase. These systems possess a continuous symmetry which is not a symmetry of the ground state, but commutes with the Hamiltonian. This effect is called spontaneous symmetry breaking.

for $t > t'$ and an analogous expression for $t < t'$. The numerator of (15) is written now in a very transparent form. At the right, one starts with the (known!) ground state $|0\rangle$, which evolves in time from $-\infty$ to t', then an electron in state λ is added. The resulting many-particle state evolves in time till t, where an electron in the same state λ is removed. The new many-particle state then evolves in time until ∞ and is eventually projected onto the ground state $|0\rangle$. The denominator just represents a phase making the right hand side of (15) equal to the left hand side if the c-operators on both sides of the equation are removed.

Condensing again the notation by introducing the time-ordering operator, we can collect the 3 S-matrices in the expression above (note that $S(t, t')$ is a bosonic operator) and eventually arrive at

$$G(\lambda, t-t') = -i\frac{\langle 0|T\{c_\lambda(t)c_\lambda^+(t')S(\infty,-\infty)|0\rangle}{\langle 0|S(\infty,-\infty)|0\rangle} \tag{16}$$

which is the form of the Green's function used as the starting point for the perturbation theory. We note again that the operators in (16) are understood to be in the interaction representation. The state $|0\rangle$ is the ground state of H_0.

In the form (16), all the nontrivialities are hidden in the S-matrix, which can be written easily as a power series in the perturbation V as was done with $U(t)$ in (13). All other elements of (16), the single-particle wave functions used in the definition of the c-operators, the ground state $|0\rangle$ of H_0, and the dynamics of the c-operators is given by the nonperturbed part H_0 of the Hamiltonian.

The only difficulty in (16) is the S-matrix in the denominator, which can be written as a power series in the perturbation V. We will see later, that the expectation value in the denominator of the Green's function will cancel some terms arising in the series expansion of the S-matrix in the numerator, and therefore poses no problem.

5 The bare electron Green's function

As an example for a Green's function, we calculate the *bare electron Green's function*, which is the Green's function for the case of a vanishing perturbation $V = 0$. This case is particularly important, because the perturbation theory will eventually give rise to a rule for the calculation of the Green's function for the nontrivial case $V = 0$ from the bare Green's function $G^{(0)}(\lambda, t-t')$ and the perturbation V.

We use Eq. (16) as a starting point for the calculation and note that a vanishing perturbation V implies that the S-matrix becomes the unit matrix. The bare Green's function, then, is given by the expression

$$G(\lambda, t-t') = -i\langle 0|T\{c_\lambda(t)c_\lambda^+(t')\}|0\rangle \equiv G^{(0)}(\lambda, t-t') \ . \qquad (17)$$

We distinguish now two main cases for the ground state of the many-electron system. The first is given by a system allowing for a varying number of particles, or, resulting in the same bare Green's function, one electron in an otherwise *empty band*. Then the ground state is the vacuum containing no particles at all. The other—and more frequent—case is the one of a *degenerate electron gas* which is a model for a metal or a heavily doped semiconductor.[5] These systems contain a large but fixed number of electrons, and therefore the ground state, called *Fermi sea* $|\mathrm{FS}\rangle$, is the state with the lowest energy for a fixed number of N particles and may be represented by the Fermi surface which separates the occupied from unoccupied states in k-space. We are talking here about the ground state $|0\rangle$ of the unperturbed system H_0. A Fermi surface, though, also exists in many systems exhibiting particle-particle interactions. In spherical systems, the Fermi surface is a sphere of radius k_F in k-space. The Fermi sea plays the role of the vacuum state for a degenerate electron gas.

5.1 An empty band

For the case of a system with a varying number of particles, the bare Green's function is particularly simple. The electron destruction operator $c_\lambda(t)$ applied to the ground state $|0\rangle$ (which corresponds to the particle vacuum) always gives zero. As a consequence, the bare Green's function (17) vanishes identically for the case $t < t'$. For $t > t'$, the creation operator is applied to the ground state resulting in the state $c_\lambda^+|0\rangle$ which has an energy of ϵ_λ. The expectation value $\langle 0|c_\lambda c_\lambda^+|0\rangle$ turns out to be one, and hence the bare Green's function is given by

$$G^{(0)}(\lambda, t-t') = -i \cdot \theta(t-t') \cdot e^{-i\epsilon_\lambda (t-t')} \ . \qquad (18)$$

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[5] Doped in such a way that at least the dopant wave functions overlap, and therefore create a band rather that isolated levels.

Perturbation theory usually is formulated in k-space rather that in real space, so we also will give the Fourier transform of the bare Green's function defined by

$$G(\lambda,\omega)=\int_{-\infty}^{\infty}dt\,e^{i\omega t}G(\lambda,t)\ . \tag{19}$$

This integral, however, does not converge for the bare Green's function $G^{(0)}$ defined in (18). Hence, we are forced to introduce a convergence factor $\exp(-\delta t)$ with $\delta=0^+$ to the exponential function in the integrand of (19). Because of the fact that the bare Green's function vanishes for negative times, this guarantees the existence of the Fourier transform, which becomes

$$G^{(0)}(\lambda,\omega)=\frac{1}{\omega-\epsilon_\lambda+i\delta}$$

and is just a simple pole in the lower half of the complex frequency plane at $\omega=\epsilon_\lambda$. *The poles of the Green's function corresponds to the excitation energies of the system.*

5.2 The degenerate electron gas

We already mentioned that the filled Fermi sea $|\mathrm{FS}\rangle$ plays the role of the vacuum state for a degenerate electron gas. When working with this ground state, it is important to consider that an electron $\boldsymbol{k}$ can only be added to the ground state, if $|\boldsymbol{k}|>k_F$. In the other case $|\boldsymbol{k}|<k_F$, an electron can only be removed from the Fermi sea. This removal can be considered as the creation of a *hole*. The removal of an electron $\boldsymbol{k}\sigma$ removes a momentum $\boldsymbol{k}$ and a spin σ as well as the energy $\epsilon_{\boldsymbol{k}}$ from the system. The creation of the hole has to have the same effect with respect to these quantities, therefore we conclude that the hole has a momentum, spin, and energy $-\boldsymbol{k}$, $-\sigma$, and $-\epsilon$, respectively.

Let us focus now the evaluation of the Green's function (17). We consider the case $t>t'$, call the energy of the Fermi sea E_0, and conclude from

$$\langle 0|e^{iH_0t}c_{\boldsymbol{k}}e^{-iH_0(t-t')}c^+_{\boldsymbol{k}}e^{-iH_0t'}|0\rangle=\langle 0|e^{iE_0t}c_{\boldsymbol{k}}e^{-i(E_0+\epsilon_{\boldsymbol{k}})(t-t')}c^+_{\boldsymbol{k}}e^{-iE_0t'}|0\rangle$$

and the fact that the operator $c^+_{\boldsymbol{k}}$ can create an electron only above the Fermi surface, that

$$G^{(0)}(\boldsymbol{k},t-t')=-ie^{-i\epsilon_{\boldsymbol{k}}(t-t')}\Theta(k-k_F)\ .$$

For the case $t < t'$, we can carry out a similar calculation or simply infer the Green's function from that for $t > t'$ while taking into account that we have to (1) exchange t and t', (2) put an overall minus sign for the exchange of the operators, (3) exchange $\epsilon_{\boldsymbol{k}}$ by $-\epsilon_{\boldsymbol{k}}$, because an electron is removed now, and (4) replace $\Theta(k-k_F)$ by $\Theta(k_F-k)$, because electrons can only be removed below the Fermi surface. Combining the result obtained in this manner with that obtained above, the Green's function for the degenerate electron gas becomes

$$G^{(0)}(\boldsymbol{k}, t-t') = -i[\Theta(t-t')\Theta(k-k_F) - \Theta(t'-t)\Theta(k_F-k)]e^{-i\epsilon_{\boldsymbol{k}}(t-t')} \ ,$$

and performing the Fourier transformation of the function in time-space yields the expression

$$G^{(0)}(\boldsymbol{k}, \omega) = \frac{1}{\omega - \epsilon_{\boldsymbol{k}} + i\delta\,\mathrm{sign}(k-k_F)} \tag{20}$$

which has a pole in the lower frequency planes for energies above the Fermi surface and pole in the upper half plane for energies below the Fermi surface.

It is often very practical to measure the energy of the electrons in the degenerate electron gas with respect to the Fermi surface. We therefore try to modify the formalism used so far in such a way that instead of the energy $\epsilon_{\boldsymbol{k}}$ the energy $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$ measured with respect to the chemical potential μ (which depends on the particle number N) appears. A simple redefinition of the energy scale, however, is only possible if we restrict ourselves to particle-number conserving excitations. In the more general case, we use a new representation of many-body theory, in which not anymore the particle number N, but the chemical potential μ is given. Then, the exact ground state is no longer determined by minimizing $\langle \mathrm{GS}|H|\mathrm{GS}\rangle$ while keeping $\langle \mathrm{GS}|N|\mathrm{GS}\rangle$ constant. Instead, the expression $\langle \mathrm{GS}|H-\mu N|\mathrm{GS}\rangle$, when minimized, gives a μ-dependent state $|\mu\rangle$ which corresponds to the exact ground state, if we put the chemical potential μ determined by the condition $\langle\mu|N|\mu\rangle = N_0$.

Then, in the definition of the Green's function $G(t)$ the operator H_0 giving the time-dependence of the c-operators is replaced by the combination $H_0 - \mu N$. Taking into consideration that the particle number commutes with the Hamiltonian H_0, it can be seen that the Green's function $G_{(\mu)}(t)$ defined for a fixed chemical potential is connected to the one defined for a fixed number of particles by the relation $G_{(\mu)}(t) = G(t) \cdot \exp i\mu t$. In the Fourier representation, therefore, the frequency ω in the expression for $G(\omega)$ has to be replaced by $\omega + \mu$ in order to get $G_{(\mu)}(\omega)$. Then, using the energy $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$ measured relatively to the Fermi energy, the expression

$$G^{(0)}_{(\mu)}(\boldsymbol{k}, \omega) = \frac{1}{\omega - \xi_{\boldsymbol{k}} + i\delta \operatorname{sign} \xi_{\boldsymbol{k}}} \tag{21}$$

results for the bare Green's function of a degenerate electron gas for a fixed chemical potential μ.

We see that the Green's function in frequency-space has a particularly simple form: for a given momentum $\boldsymbol{k}$ it consists of a simple pole (of residue 1) at the single-particle excitation energy $\xi_{\boldsymbol{k}}$. In order to describe electrons ($\xi_{\boldsymbol{k}} > 0$) and holes ($\xi_{\boldsymbol{k}} < 0$) with one single Green's function, the pole, if related to an electron, is located in the lower frequency half plane. If related to a hole, the pole is in the upper half of the complex frequency plane.

6 Perturbative evaluation of the Green's function

6.1 Expansion of the S-matrix

For the purpose of evaluating the Green's function, we are going to focus on its numerator of (16). We expand the S-matrix in a series in the perturbation V using (14). Then, a typical term in the expansion looks like

$$\frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \, \langle 0 | T\{c_\lambda(t) c^+_\lambda(t') V(t_1) \cdots V(t_n)\} | 0 \rangle \; . \tag{22}$$

The perturbation V in general will always consist of a number of electron creation and annihilation operators, and also of operators creating and annihilating other elementary excitations. We give two examples. In the first example, the *Coulomb interaction* only involves electronic excitations. Two electrons take part in the Coulomb interaction, therefore, two creation and two annihilation operators will come into the game. In the Schrödinger representation, the interaction is given by (8). In the interaction representation all four operators in the Coulomb interaction are taken at the same time.

The second example is the *electron-phonon interaction* which is represented by the equation

$$V = \sum_{\boldsymbol{q},\boldsymbol{k}} M^{\lambda,n,n'}_{\boldsymbol{q},\boldsymbol{k}} c^+_{n',\boldsymbol{k}+\boldsymbol{q}} c_{n,\boldsymbol{k}} (a_{\boldsymbol{q}\lambda} + a^+_{-\boldsymbol{q}\lambda}) \tag{23}$$

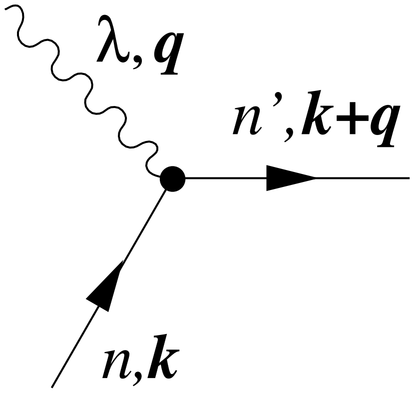

Figure 3: The electron-phonon interaction.

which describes the annihilation of a phonon of momentum $\boldsymbol{q}$ and branch index λ (by the operator $a_{\boldsymbol{q}\lambda}$) while scattering an electron from band n and momentum $\boldsymbol{k}$ to band n' and momentum $\boldsymbol{k}+\boldsymbol{q}$ (see Fig. 3). This electron scattering process may also be related to the creation of a phonon with momentum $-\boldsymbol{q}$ and branch index λ (given by the operator $a^{+}_{-\boldsymbol{q}\lambda}$). Both processes have the same amplitude which is given by $M^{\lambda,n,n'}_{\boldsymbol{q},\boldsymbol{k}}$. Therefore, the two phonons under discussion are usually considered to be one phonon excitation by introducing the operator $A_{\boldsymbol{q}\lambda} = a_{\boldsymbol{q}\lambda} + a^{+}_{-\boldsymbol{q}\lambda}$. The transition to the interaction representation is performed again by writing the three operators in former equation in the interaction representation individually.

From the discussion given above, we conclude that the ground state expectation value in (22) can be considered for all practical purposes as consisting of an equal number of electron creation and destruction operators, taken at particular times, in the interaction representation and creation and destruction operators of other excitations, for instance phonon excitations. As a matter of fact, operators to different excitation types commute. Therefore the time-ordered product of a collection of, say, electron creation and destruction operators and phonon operators is equal to the time-ordered product of the electron operators times the time-ordered product of the phonon operators. The expectation value of this product can be separated into an expectation value of electron operators times an expectation value of phonon operators, respectively. Hence, we are going to discuss the ground state expectation value of the time-ordered product of a collection of m electron creation and m electron annihilation operators.

6.2 Time-ordering, pairing, and Wick's theorem

The expectation values of time-ordered products of creation and destruction operators like the one in (22) with V from (23) involve considerable complexity due to the presence of the time-ordering operator. A number of $2m$ operators, taken at different times, allows for up to $(2m)!$ different time-orderings. Fortunately, most of these ordered products vanish, and the time-ordering can be reformulated in a relatively simple manner. This reformulation is based on Wick's theorem. Before stating the theorem, we introduce some concepts which are important for its application.

Consider the expectation value

$$\langle 0|T\{c_\alpha(t_\alpha)c_\beta^+(t_\beta)c_\gamma(t_\gamma)c_\delta^+(t_\delta)\}|0\rangle \ . \tag{24}$$

We assume a certain relation for the time arguments, say $t_\delta > t_\alpha > t_\gamma > t_\beta$, and perform the time-ordering. This leads to

$$+\langle 0|c_\delta^+ c_\alpha c_\gamma c_\beta^+|0\rangle$$

(we suppress the time arguments from now on). The term has a positive sign because an even number of 4 transpositions is needed for the reordering of the operators.

The concept of *pairing* is based on the following observation. The operator c_β^+ adds an electron in state β to the ground state. If this electron is not removed later on, the expectation value above will vanish. In other words, either α has to be equal to β, or γ has to be equal to β. For all other cases, the expectation value vanishes. This yields

$$\langle 0|c_\gamma^+ c_\alpha c_\gamma c_\alpha^+|0\rangle \delta_{\alpha\beta}\delta_{\gamma\delta} + \langle 0|c_\alpha^+ c_\alpha c_\beta c_\beta^+|0\rangle \delta_{\alpha\delta}\delta_{\beta\gamma} \ , \tag{25}$$

and the number of two terms in this expression reflects the fact that there are two possibilities to pair two creation operators with two destruction operators. A product of m creation and m annihilation operators allows for $m!$ different pairings.

The operators in expression (25) may be regrouped. This *regrouping* is done in such a way that the ordering of operators to the same states is not altered because this would produce an extra term according to $\{c, c^+\} = 1$.

Again we take into account that an odd number of transpositions of the operators yields a minus sign, and arrive at the expression

$$-\langle 0|c_\gamma^+ c_\gamma c_\alpha c_\alpha^+|0\rangle \delta_{\alpha\beta}\delta_{\gamma\delta} + \langle 0|c_\alpha^+ c_\alpha c_\beta c_\beta^+|0\rangle \delta_{\alpha\delta}\delta_{\beta\gamma}\ .$$

Note that in the first term of this expression, first an electron in state α is created, and subsequently removed. After the removal of this electron, we are back in the ground state, because the creation and destruction operators are creating and annihilating electrons in the eigenstates of H_0, and the ground state is meant to be the ground state of H_0. The dynamics added when introducing the interaction representation is the dynamics which is caused by the Hamiltonian H_0 also. Therefore, the electron created in state α will stay in this state. Hence, the expectation values in the equation above can be split into expectation values of products of one creation and one destruction operator,

$$\langle 0|c_\gamma^+ c_\gamma|0\rangle\langle 0|c_\alpha c_\alpha^+|0\rangle \delta_{\alpha\beta}\delta_{\gamma\delta} - \langle 0|c_\alpha^+ c_\alpha|0\rangle\langle 0|c_\beta c_\beta^+|0\rangle \delta_{\alpha\delta}\delta_{\beta\gamma}\ .$$

This is equivalent to (24) for the given time relation. The ground state expectation values only contain products of a creation and a destruction operator and, therefore, are very similar to the known bare Green's function. *Wick's theorem expresses expectation values of the form (24) as sums of products of bare Green's functions.*

Wick's theorem can be stated in the form of a handy rule:

- To calculate an expectation value of a time-ordered product of m creation and m annihilation operators, add all possible different pairings of creation and annihilation operators which amount to $m!$.
- To *pair* a creation and a annihilation operators means to bring them together (the annihilation operator to the left of the creation operator) by repeated transpositions while taking care of the sign. Then replace the pair by the time-ordered ground state expectation value of the pair.

For a proof of Wick's theorem, refer to [3], Sect. 8.2.

After having applied Wick's theorem, the expectation value under consideration is expressed as a sum of products made up of the factors

$$\begin{aligned}&\langle 0|T\{c_\lambda(t)c_{\lambda'}^+(t')\}|0\rangle = \\ &\quad = \delta_{\lambda\lambda'} \times \begin{cases} iG^{(0)}(\lambda, t-t') & \text{for } t \neq t' \\ -\langle 0|c_\lambda^+(t)c_\lambda(t)|0\rangle = -\theta(\xi_\lambda - \xi_F) & \text{for } t = t'\ . \end{cases}\end{aligned} \tag{26}$$

Sometimes, the Fermi function $n_F(\xi_\lambda) = n_F(\epsilon_\lambda - \mu)$ is used instead of the factor $\theta(-\xi_\lambda)$. For $T = 0$ formalism, this is exactly the same.

6.3 Feynman diagrams

As an example we calculate the numerator of the Green's function for the system $H = H_0 + V$ where H_0 is the Hamiltonian of the free Fermi gas (7), and V is the electron-phonon coupling mentioned above. We shall consider only one phonon branch, one electronic band, and a electron-phonon matrix element independent of the electron momentum $\boldsymbol{k}$, that is

$$V = \sum_{\boldsymbol{q}} M_{\boldsymbol{q}} c^+_{\boldsymbol{k}+\boldsymbol{q}} c_{\boldsymbol{k}} A_{\boldsymbol{q}} \tag{27}$$

with $A_{\boldsymbol{q}} = a_{\boldsymbol{q}} + a^+_{-\boldsymbol{q}}$. The contribution of nth order in the perturbation V to the numerator of the Green's function is given by (22). It is obvious that the contribution of zeroth order in V leads to the bare Green's function $G^{(0)}$. Furthermore, the contribution to the Green's function of first order in the perturbation V vanishes, because the expectation values of one phonon operator $\langle 0|A_{\boldsymbol{q}\lambda}|0\rangle$ are equal to zero. Hence we focus on the contribution of second order in V. Taking care on the prefactor, this reads

$$(-i) \cdot \frac{(-i)^2}{2!} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \, \langle 0|T\{c_{\boldsymbol{k}}(t) V(t_1) V(t_2) c^+_{\boldsymbol{k}}(t')\}|0\rangle \; . \tag{28}$$

By replacing the perturbation V in the interaction representation into (28), and separating phonon operators from electron operators we find

$$\begin{aligned} \frac{(-i)^3}{2!} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \sum_{\boldsymbol{q}_1,\boldsymbol{q}_2} M_{\boldsymbol{q}_1} M_{\boldsymbol{q}_2} \langle 0|T\{A_{\boldsymbol{q}_1}(t_1) A_{\boldsymbol{q}_2}(t_2)\}|0\rangle \times \\ \times \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \langle 0|T\{c_{\boldsymbol{k}}(t) c^+_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1) c_{\boldsymbol{k}_1}(t_1) c^+_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2) c_{\boldsymbol{k}_2}(t_2) c^+_{\boldsymbol{k}}(t')\}|0\rangle \; . \end{aligned} \tag{29}$$

The first expectation value in this expression can be written in terms of the (bare) phonon Green's function $D^{(0)}(\boldsymbol{q}, t_1 - t_2)$

$$i\delta_{\boldsymbol{q}_1+\boldsymbol{q}_2,0} D^{(0)}(\boldsymbol{q}_1, t_1 - t_2) \; ,$$

where $D^{(0)}(\boldsymbol{q}, t_1 - t_2)$ is defined as

$$D^{(0)}(\boldsymbol{q}, t_1 - t_2) = -i\langle 0|T\{A_{\boldsymbol{q}}(t_1) A_{-\boldsymbol{q}}(t_2)\}|0\rangle \; . \tag{30}$$

The phonon Green's function will be discussed later in this appendix. The second expectation value has to be decomposed into combinations of the bare electron Green's function by making use of Wick's theorem. We find the $3! = 6$ different pairings[6]

$$\begin{aligned}
&\langle T\{c_{\boldsymbol{k}}(t)c^{+}_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1)c_{\boldsymbol{k}_1}(t_1)c^{+}_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2)c_{\boldsymbol{k}_2}(t_2)c^{+}_{\boldsymbol{k}}(t')\}\rangle \\
&= \langle T\{c_{\boldsymbol{k}}(t)c^{+}_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_1}(t_1)c^{+}_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_2}(t_2)c^{+}_{\boldsymbol{k}}(t')\}\rangle \\
&+ \langle T\{c_{\boldsymbol{k}}(t)c^{+}_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_2}(t_2)c^{+}_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_1}(t_1)c^{+}_{\boldsymbol{k}}(t')\}\rangle \\
&- \langle T\{c_{\boldsymbol{k}}(t)c^{+}_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_1}(t_1)c^{+}_{\boldsymbol{k}}(t')\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_2}(t_2)c^{+}_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2)\}\rangle \\
&+ \langle T\{c_{\boldsymbol{k}}(t)c^{+}_{\boldsymbol{k}}(t')\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_1}(t_1)c^{+}_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_2}(t_2)c^{+}_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2)\}\rangle \\
&+ \langle T\{c_{\boldsymbol{k}}(t)c^{+}_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_1}(t_1)c^{+}_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_2}(t_2)c^{+}_{\boldsymbol{k}}(t')\}\rangle \\
&- \langle T\{c_{\boldsymbol{k}}(t)c^{+}_{\boldsymbol{k}}(t')\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_1}(t_1)c^{+}_{\boldsymbol{k}_2+\boldsymbol{q}_2}(t_2)\}\rangle \cdot \langle T\{c_{\boldsymbol{k}_2}(t_2)c^{+}_{\boldsymbol{k}_1+\boldsymbol{q}_1}(t_1)\}\rangle \;.
\end{aligned} \tag{31}$$

Note again that expectation values have been ordered such that the creation operator is placed to the right of the destruction operator, and in addition, a time ordering operator has been added. The expectation values in (31) can be expressed as bare Green's functions or as a Fermi function n_F according to (26). Performing this step and noting that the factor $\delta_{\boldsymbol{q}_1+\boldsymbol{q}_2,0} = 0$ is already present in (29), we obtain

$$\begin{aligned}
&(\mathrm{a}) = i^3\delta_{\boldsymbol{k},\boldsymbol{k}_1+\boldsymbol{q}_1}\delta_{\boldsymbol{k}\boldsymbol{k}_2}G^{(0)}(\boldsymbol{k},t-t_1)G^{(0)}(\boldsymbol{k}-\boldsymbol{q}_1,t_1-t_2)G^{(0)}(\boldsymbol{k},t_2-t') \\
&(\mathrm{b}) = i^3\delta_{\boldsymbol{k}\boldsymbol{k}_1}\delta_{\boldsymbol{k},\boldsymbol{k}_2-\boldsymbol{q}_1}G^{(0)}(\boldsymbol{k},t-t_2)G^{(0)}(\boldsymbol{k}+\boldsymbol{q}_1,t_2-t_1)G^{(0)}(\boldsymbol{k},t_1-t') \\
&(\mathrm{c}) = i^2\delta_{\boldsymbol{k}\boldsymbol{k}_1}\delta_{\boldsymbol{q}_1,0}n_F(\xi_{\boldsymbol{k}_2})G^{(0)}(\boldsymbol{k},t-t_1)G^{(0)}(\boldsymbol{k},t_1-t') \\
&(\mathrm{d}) = i\delta_{\boldsymbol{q}_1,0}n_F(\xi_{\boldsymbol{k}_1})n_F(\xi_{\boldsymbol{k}_2})G^{(0)}(\boldsymbol{k},t-t') \\
&(\mathrm{e}) = i^2\delta_{\boldsymbol{q}_1,0}\delta_{\boldsymbol{k}\boldsymbol{k}_2}n_F(\xi_{\boldsymbol{k}_1})G^{(0)}(\boldsymbol{k},t-t_2)G^{(0)}(\boldsymbol{k},t_2-t') \\
&(\mathrm{f}) = -i^3\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2-\boldsymbol{q}_1}G^{(0)}(\boldsymbol{k},t-t')G^{(0)}(\boldsymbol{k}_1,t_1-t_2)G^{(0)}(\boldsymbol{k}_1+\boldsymbol{q}_1,t_2-t_1)
\end{aligned} \tag{32}$$

The terms have been written in the same order as in the equation above. Some of the Kronecker δ-functions in (32) drop out, because they identically vanish.

This expression is still rather cumbersome but fortunately it can be expressed by physically very intuitive diagrams, the *Feynman diagrams*. In the time domain the rules for associating a Feynman diagram to an expression like one of the six above are as follows. Each bare Green's function

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[6] we have shortened a bit the notation writing $\langle\cdots\rangle$ as an abbreviation for $\langle 0|\cdots|0\rangle$.

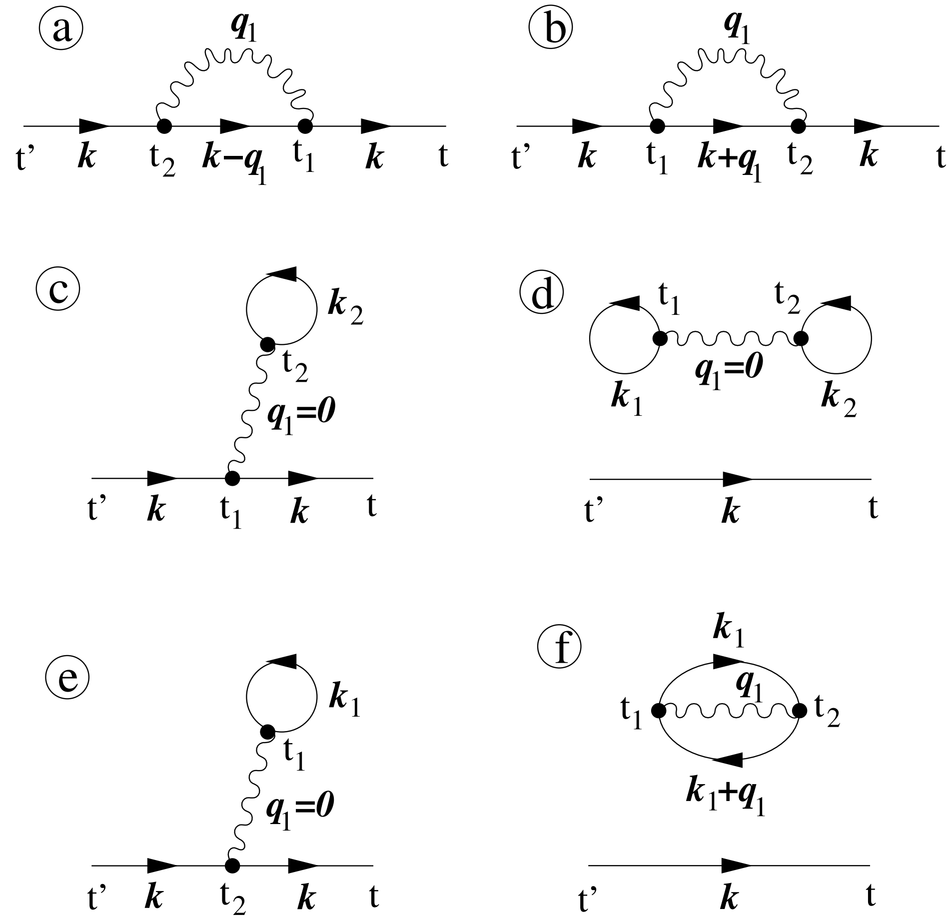

Figure 4: Feynman diagrams for the renormalization of the electron Green's function by phonons to second order in the electron-phonon coupling matrix element.

$G^{(0)}(\boldsymbol{k}, t-t')$ is represented by a small straight line carrying a quasimomentum $\boldsymbol{k}$ and reaching from the time t' to t. The line also includes an arrow denoting a direction. The meaning of this arrow will be explained later. It does *not* imply that $t' < t$. Nor does it imply that the line represents an electron if the arrow points from left to right and a hole, if it points from right to left. A Green's function with $t = t'$, that is, a factor n_F, is represented by a small circle. The direction of the line forming the circle is arbitrary and has no consequences.

A phonon is represented by a wavy line. It does not carry an arrow because the phonon Green's function is even in the time argument. The representations of the Coulomb interaction and also of photons will be given later. We can already surmise that the representation of photons (also other bosons) will be isomorphic to that of phonons.

We discuss now the 6 diagrams of Fig. 4), starting with the one denoted by (a) and construct its associated Feynman diagram. The third Green's function from the left in expression (a) of (32) represents an electron propagating from t' to t_2 and having a quasimomentum of $\boldsymbol{k}$. We denote it by a line from t' to t_2 with a label $\boldsymbol{k}$. At the time T_2 two things happen. First, the electrons continues propagating, from t_2 to t_1, with a momentum of $\boldsymbol{k} - \boldsymbol{q}_1$. Second, a phonon carrying the missing $\boldsymbol{q}_1$ is created. We draw an electron line to t_1 and start a new wavy phonon line at t_2. At t_1, the phonon is destroyed, and the electron continues to propagate with its initial momentum $\boldsymbol{k}$ to t. The contribution of this diagram to the numerator of the Green's function (the term (29)) is given by the term

$$\begin{aligned} &\frac{i}{2!}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \sum_{\boldsymbol{q}} |M_{\boldsymbol{q}}|^2 D^{(0)}(\boldsymbol{q}, t_1 - t_2)\times \\ &\quad\times G^{(0)}(\boldsymbol{k}, t-t_1) G^{(0)}(\boldsymbol{k}-\boldsymbol{q}, t_1-t_2) G^{(0)}(\boldsymbol{k}, t_2 - t')\ , \end{aligned} \tag{33}$$

it has to be taken into account that $M_{-\boldsymbol{q}} = M^*_{\boldsymbol{q}}$. The nodes at t_1 and t_2 in the diagram in Fig. 4(a) are called *vertices* and are related to the electron-phonon matrix element $M_{\boldsymbol{q}}$. One of the vertices represents the creation of a phonon, the other the destruction of a phonon. Therefore, the matrix element $M_{\boldsymbol{q}}$ appears as a complex conjugated pair: the matrix element for a time reversed process is the complex conjugate of that for the direct process.

In the diagram, the quasimomentum $\boldsymbol{q}$ is summed over. In this way all possible phonons are included. The time integrations show that the way a diagram is drawn or the arrows are put on the electron lines does not imply any time ordering. The arrows denote *particle number conservation* at the vertices.

The diagram in Fig. 4(b) is very similar to that in Fig. 4(a). The only difference is the labeling of some of the variables. It can be shown that there are always $n!$ diagrams in the nth order perturbation contribution which are equal in the sense that their contribution to the Green's function is the same. The related diagrams then are called *topologically equal*, which means that by relabeling internal variables, the diagrams become identical. When using perturbation theory one only draws one representative of these $n!$ topologically identical diagrams, and removes the factor $1/n!$ in the corresponding perturbation term.

Let us proceed with the diagram Fig. 4(c). This time we have an electron propagating from t' to t_1, and then from t_1 to t. In both cases it carries a quasimomentum $\boldsymbol{k}$. At the time t_1, a phonon is created. Because of the factor $\delta_{\boldsymbol{q}_1,0}$ in the expression for the diagram (c), this must be a Γ-point phonon. At t_2 this phonon is destroyed. Correspondingly, the factor $n_F(\xi_{\boldsymbol{k}_2})$ appears. We recall the fact that this is a Green's function with the time argument $t_1 - t_1$. Therefore we draw this factor as a loop formed by an electron line. The loop is attached to the time t_1 (and similarly to t_2).

The diagrams (d) and (e) are constructed in a similar manner, and also contain a Γ-point phonon. This phonon has no dynamics,[7] it corresponds to static strain which is meant to be not included in the Hamiltonian H. Therefore, they vanish.

The last expression is represented by diagram (f). We start with its first Green's function which denotes an electron traveling from t' to t. At t_1, an electron with momentum $\boldsymbol{k}_1$ and a phonon with quasimomentum $\boldsymbol{q}_1$ are created. Furthermore, an electron with quasimomentum $\boldsymbol{k}_1 + \boldsymbol{q}_1$ is destroyed. This is necessary to conserve particle number and the quasimomentum. At time t_2 a similar annihilation happens.

Note that the diagrams (d) and (f) have a very particular property: they decay into separable, independent parts. Diagram (f), for instance, is just given by a bare Green's function $G^{(0)}(\boldsymbol{k}, t - t')$ times some factor. It can be shown that the contributions arising from these separable parts, whose related diagrams are called *disconnected* diagrams, exactly cancel the factor $\langle 0|S(\infty, -\infty)|0\rangle$ in the denominator of the Green's function.

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[7] This is only true for acoustic phonons, but not for optical phonons.

6.4 Reformulation in the frequency-domain

Before concluding this section and stating the Feynman rules, which tell how to determine the contributions of nth order perturbation theory to the Green's function, we write the diagrams and their corresponding mathematical expressions in the frequency domain by performing a Fourier transformation of the Green's function. It will turn out that this introduces a further simplification in the perturbation series for the Green's function. We have seen in the paragraphs above (refer, e.g., to (33)) that the time integrals over the products of Green's function have the form of a convolution; the individual Green's functions in the integrand depend on time via differences $t_i - t_{i+1}$. By expressing the calculations in the frequency domain, these convolutions become simply products.

How this Fourier transformation is performed, and what implications it has, will be explained using as an example the contribution shown in Fig. 4(a) to the Green's function, or, respectively, Eq. (33). In this expression, we replace the Green's functions by the corresponding frequency-dependent Green's functions

$$G(\boldsymbol{k}, t - t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G(\boldsymbol{k}, \omega) \ ,$$

and similarly for the phonon Green's function. This introduces the four factors $\exp -i\nu(t_1 - t_2)$, $\exp -i\omega(t - t_1)$, $\exp -i\omega'(t_1 - t_2)$, and $\exp -i\omega''(t_2 - t')$ for the bare phonon and the first, second, and third bare electron, respectively. Collecting all these terms together, the time dependent part of (33) becomes

$$\int dt_1 \int dt_2 \, e^{-i\omega t} e^{-i(\omega'+\nu-\omega)t_1} e^{-i(\omega''-\nu-\omega')t_2} e^{i\omega'' t'}$$

which, when integrated, gives rise to the two δ-functions $2\pi\delta(\omega' + \nu - \omega)$ and $2\pi\delta(\omega'' - \nu - \omega')$ which guarantee the conservation of energy at the *vertices* (the vertices correspond to the nodes in the Feynman diagram, places where 2 or more lines are joined) and remove the integrals over the internal frequencies ω' and ω'' introduced by the Fourier transformation. Then, only the factor $exp(-i\omega(t - t'))$ is left which resembles the one in the Fourier transformation of the whole expression (33). The diagram given in Fig. 4(a) corresponds consequently to the diagram in Fig. 5 when working in frequency space, whereas the corresponding contribution to the frequency-dependent

Green's function becomes

$$\frac{i}{2!}\sum_{\boldsymbol{q}} |M_{\boldsymbol{q}}|^2 G^{(0)}(\boldsymbol{k},\omega)\left[\int \frac{d\omega}{2\pi}\,D^{(0)}(\boldsymbol{q},\nu)G^{(0)}(\boldsymbol{k}-\boldsymbol{q},\omega-\nu)\right]G^{(0)}(\boldsymbol{k},\omega)\ . \tag{34}$$

Comparing this expression to the diagram in Fig. 5, we notice some important points related to Feynman diagrams. (i) the *incoming* and the *outgoing* bare Green's functions which carry the same indices as the Green's function $G(\boldsymbol{k},\omega)$ to which they contribute. This is clearly related to (ii), the conservation of quasimomentum and energy (i.e. frequency) at each of the vertices of the diagram. For the case of the two quasimomenta, this conservation was already introduced when building pairs according Wick's theorem, and ultimatively are a consequence of the translational invariance of the system under consideration (here it does not matter whether there is a "full" continuous translation like the translation group of space, or "only" discrete translations like those imposed by a Bravais lattice). The conservation of energy was introduced when performing the Fourier transformation, and relates to the fact that the Green's function is a function of time *differences* only.

(iii) All internal lines (i.e. all lines but the incoming and outgoing ones) are given *internal* quantum numbers (i.e. $\boldsymbol{q}$), which only have to satisfy the momentum and frequency conservation at each vertex. If many possibilities are compatible with this constraint, they are summed over as in the case of (34) for the variables $\boldsymbol{q}$ and ω.

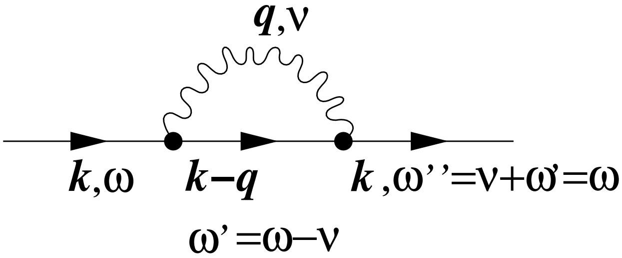

Figure 5: A Feynman diagram in frequency space.

6.5 A conclusion: the Feynman rules

In addition to introducing the Feynman diagrams, the example above has demonstrated some basic principles. The first is the cancellation of the ground state expectation value of the S-matrix. Those terms in the numerator of the Green's function (16) which correspond to *nonconnected* diagrams exactly cancel the denominator in (16). The second one deals with the *topologically equivalent* Feynman diagrams. The nth order (in V) term in the numerator of the Green's function yields $n!$ Feynman diagrams which are topologically equivalent, that is just differ by a different labeling of integration (or sum) variables.

Taking these principles into account, we can state that the Green's function is given by a formula much simpler than that in (16):

$$G(\boldsymbol{k}, t - t') = -i\langle 0|T\{c_{\boldsymbol{k}}(t)c^+_{\boldsymbol{k}}(t')S(\infty, -\infty)\}|0\rangle_{\text{diff, con}}$$

where the index "diff, con" indicates that only *topologically different* and *connected* (i.e. not disconnected) contributions are considered.

Reformulating this statement, and including the rules for drawing diagrams, we arrive at *Feynman's rules* for the calculation of the contribution to the Green's function arising as an nth order perturbation in V.

Feynman rules: When intending to calculate the contribution to the electron Green's function[8] $iG(\boldsymbol{k}, \omega)$ arising in nth order perturbation theory from electron-phonon coupling (here, $n = 2m$, all other contributions vanish), we

- draw all topologically different, connected diagrams which consist of an incoming and an outgoing bare Green's function, and contain $n/2$ internal phonon lines and $n - 1$ electron lines. To the electron lines, arrows are added which represent particle conservation at the vertices of the diagram. Then,

- the incoming and outgoing electron Green's functions are labeled with momentum $\boldsymbol{k}$ and frequency ω, and the internal lines are all also labeled with internal momentum and frequency variables taking into consideration the conservation of momentum and frequency at each of the vertices (This depends on the direction of the arrow in the case of electron lines).

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[8] Note the factor i in front of the Green's function. The rules presented here are valid for the calculation of iG, not for G.

- When translating the Feynman diagram to an analytic expression, we write $G^{(0)}(\boldsymbol{k},\omega)$ for each of the electron lines carrying labels $\boldsymbol{k},\omega$. The direction in which the arrow on the electron line points does not matter. We write $D^{(0)}(\boldsymbol{q},\nu)$ for a phonon line with labels $\boldsymbol{q},\nu$.
- Then each pair of vertices terminating phonon lines is represented by the squared electron-phonon matrix element $|M_{\boldsymbol{q}}|^2/\Omega$ (Ω is the integration volume).
- As a next step, all the internal quasimomenta are summed over and all the internal frequencies are integrated over by inserting the appropriate sums and integrals $\sum_{\boldsymbol{q}}$ and $\int d\omega/(2\pi)$.
- Finally, we put a factor $i^n(-1)^F(2S+1)^F$ where F is the number of *closed* fermion loops, and S denotes the spin quantum number of the electrons.

The last rule comes from the fact that the Green's functions actually correspond to second rank tensors in spin space and, in the simplest case of no external magnetic field and no spin-spin interactions, have the form $G_{\alpha\beta}(\boldsymbol{k},\omega)=\delta_{\alpha\beta}G(\boldsymbol{k},\omega)$. When evaluating the diagram obviously a sum over the spin indices has to be carried out. And in Fermion loops, combinations like $\delta_{\alpha\alpha}G$ or $\delta_{\beta\gamma}G\delta_{\gamma\beta}G$ yield a factor of $2S+1$ when the spin sum is performed.

6.6 The bare phonon Green's function

We close this section by calculating explicitly the bare phonon Green's function defined in (30). The phonon operators $A_{\boldsymbol{q}}$ are given by $A_{\boldsymbol{q}} = a_{\boldsymbol{q}} + a^+_{-\boldsymbol{q}}$ (when suppressing the branch index λ). When evaluating the product $A_{\boldsymbol{q}}(t_1)A_{-\boldsymbol{q}}(t_2)$ we first restrict to the case $t_1 > t_2$ to circumvent the difficulty presented by the time-ordering operator. The other case works similarly and has to be taken into account when formulating the result of the calculation given here. The evaluation of the product above consisting of two A-operators, yields four combinations of two a-operators each. The expectation value of the combinations consisting of creation or destruction operators only vanishes, and the terms left contain the combinations $a^+_{-\boldsymbol{q}}a_{-\boldsymbol{q}}$ and $a_{\boldsymbol{q}}a^+_{\boldsymbol{q}}$. The state $|0\rangle$ here corresponds to the vacuum state of the phonon field, and therefore contains no phonon at all. Hence, the expectation value of $a^+_{-\boldsymbol{q}}a_{-\boldsymbol{q}}$ also vanishes. The time dependence of the remaining term is given by $a_{\boldsymbol{q}}(t_1)a^+_{\boldsymbol{q}}(t_2) = \exp -i\omega_{\boldsymbol{q}}(t_1 - t_2) \times a_{\boldsymbol{q}}a^+_{\boldsymbol{q}}$ and recalling the quantum theory of the harmonic oscillator then leaves us with the result

$$\begin{aligned} D^{(0)}(\boldsymbol{q}, t_1 - t_2) &= -i\langle 0|T\{A_{\boldsymbol{q}}(t_1)A_{-\boldsymbol{q}}(t_2)\}|0\rangle \\ &= -i \times \left\{ \begin{array}{ll} e^{-i\omega_{\boldsymbol{q}}(t_1-t_2)} & \text{for } t_1 > t_2 \\ e^{i\omega_{\boldsymbol{q}}(t_1-t_2)} & \text{for } t_1 < t_2 \end{array} \right. \end{aligned} \tag{35}$$

where the case $t_1 < t_2$ was taken into account already. The Fourier transformation of the bare phonon Green's function gives

$$\begin{aligned} D^{(0)}(\boldsymbol{q}, \omega) &= \frac{1}{\omega - \omega_{\boldsymbol{q}} + i\delta} - \frac{1}{\omega + \omega_{\boldsymbol{q}} - i\delta} \\ &= \frac{2\omega_{\boldsymbol{q}}}{\omega^2 - \omega^2_{\boldsymbol{q}} + i\delta} \end{aligned} \tag{36}$$

which has two poles, one at the frequency $\omega = \omega_{\boldsymbol{q}}$, slightly shifted to the lower frequency plane, and the second at $\omega = -\omega_{\boldsymbol{q}}$, slightly shifted to the upper frequency plane.

7 Self-energy contributions and the Dyson equation

In the last section, we have come to the conclusion that the contribution to the Green's function in nth order of the perturbation V in (27) is given by all topologically different and connected Feynman diagrams containing $n/2$ phonon lines. For most of the applications of Green's function theory it is still not sufficient to approximate the Green's function by its bare counterpart plus the terms given by perturbation theory up to, say, order N. Instead, important contributions to the Green's function have to be included to *all orders*.

It is important to stress that only the certain terms have to be included to infinite order. Taking all diagrams to all orders would be an insurmountable task. But the inclusion of certain important contributions[9] to all orders is relatively easy to manage by applying the *Dyson equation*.

Let us look at a simple example. The diagrams contributing to the electronic Green's function in 4th order of the electron-phonon matrix element are show in Fig. 6.

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[9] Which contributions are important is shown by "experience."

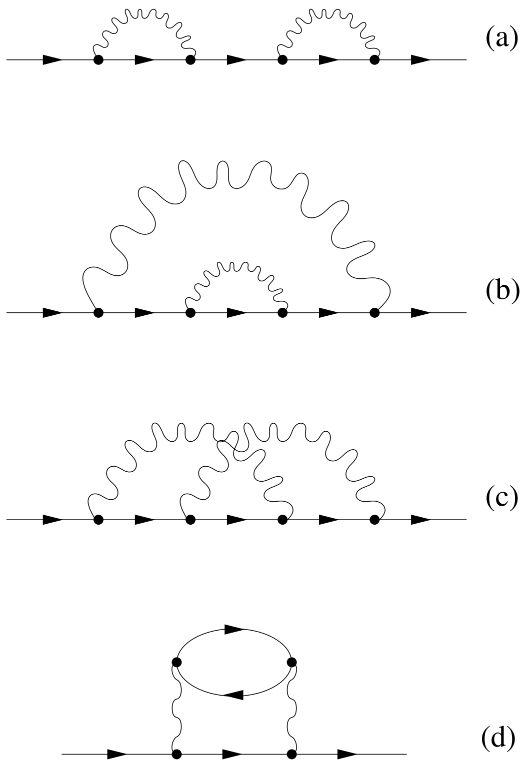

Figure 6: Feynman diagrams for the renormalization of the electron Green's function by phonons in fourth order of the electron-phonon coupling matrix element.

We focus on the diagram of Fig. 6(a). It is simply twice the diagram in Fig. 5. In sixth order perturbation theory it will occur again, then being three times the diagram in Fig. 5. Considering this class of diagrams up to infinite order is equivalent to summing a geometrical series and can be performed easily, provided it converges.

The diagram in Fig. 5 translates according to the Feynman rules into the expression

$$iG^{(0)}(\boldsymbol{k},\omega)\Sigma_1(\boldsymbol{k},\omega)G^{(0)}(\boldsymbol{k},\omega)$$

$$\text{with}\qquad \Sigma_1(\boldsymbol{k},\omega) = -\sum_{\boldsymbol{q}} |M_{\boldsymbol{q}}|^2 \int \frac{d\omega}{2\pi} D^{(0)}(\boldsymbol{q},\nu) G^{(0)}(\boldsymbol{k}-\boldsymbol{q},\omega-\nu)\ .$$

It is clear that the diagram in Fig. 6(a) then is represented by the expression

$$iG^{(0)}(\boldsymbol{k},\omega)\left[\Sigma_1(\boldsymbol{k},\omega)G^{(0)}(\boldsymbol{k},\omega)\right]^m$$

for $m = 2$. For $m = 2n > 2$ it corresponds to an m-fold repetition of Fig. 5. Summing up the contributions for all $m = 2n$ $(n = 0 \ldots \infty)$ yields

$$\begin{aligned} G_1(\boldsymbol{k},\omega) &= G^{(0)}(\boldsymbol{k},\omega) + \sum_m G^{(0)}(\boldsymbol{k},\omega)\left[\Sigma_1(\boldsymbol{k},\omega)G^{(0)}(\boldsymbol{k},\omega)\right]^m \\ &= G^{(0)}(\boldsymbol{k},\omega) + G^{(0)}(\boldsymbol{k},\omega)\Sigma_1(\boldsymbol{k},\omega)G_1(\boldsymbol{k},\omega)\ . \end{aligned} \tag{37}$$

We have denoted by $G_1(\boldsymbol{k},\omega)$ the Green's function that results from summing all the diagrams consisting of a sequence of that in Fig. 5. A graphical representation of (37) is shown in Fig. 7.

Clearly, the Green's function G_1 defined in the last paragraph is only an approximation to the exact Green's function G. But the method above can be extended to give the exact Green's function as well (at least in principle). This extension is based upon the observation that the function $\Sigma_1(\boldsymbol{k},\omega)$ can be replaced by a function $\Sigma(\boldsymbol{k},\omega)$, such that the function G_1 becomes the exact Green's function. The resulting *Dyson equation* is

$$G(\boldsymbol{k},\omega) = G^{(0)}(\boldsymbol{k},\omega) + G^{(0)}(\boldsymbol{k},\omega)\Sigma(\boldsymbol{k},\omega)G(\boldsymbol{k},\omega)\ , \tag{38}$$

where the *self energy* $\Sigma(\boldsymbol{k},\omega)$ is the sum of all *irreducible self-energy parts* $\Sigma_i(\boldsymbol{k},\omega)$. As irreducible self-energy parts we designate diagrams which can be put between two electron lines and cannot be separated into two nonconnected parts by just cutting one electron line. Equation (38) generates the whole series of diagrams contributing to the Green's function by iteration and in this manner generates all different sequences of self-energy parts Σ_i to form diagrams of higher order in the perturbation. The diagram in Fig. 6(a) is generated in the second iteration of the Dyson equation as

$$G^{(0)}(\boldsymbol{k},\omega)\Sigma_1(\boldsymbol{k},\omega)G^{(0)}(\boldsymbol{k},\omega)\Sigma_1(\boldsymbol{k},\omega)G^{(0)}(\boldsymbol{k},\omega)$$

and if the diagram related to the expression $\Sigma_1(\boldsymbol{k},\omega)G^{(0)}(\boldsymbol{k},\omega)\Sigma_1(\boldsymbol{k},\omega)$ would be included as a self-energy part Σ_2 in the self energy, the diagram in Fig. 6(a) also would be generated in the first iteration of the Dyson equation as $G^{(0)}(\boldsymbol{k},\omega)\Sigma_2(\boldsymbol{k},\omega)G^{(0)}(\boldsymbol{k},\omega)$ and would be incorrectly counted twice.

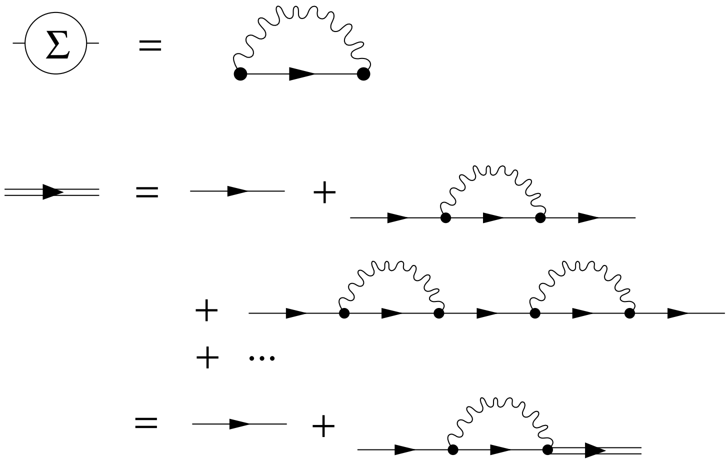

Figure 7: Self energy and Dyson equation.

The recipe usually employed to calculate the Green function is to calculate the self energy first, and then replace it into Dyson's equation. It is clear, however, that the self energy cannot be calculated exactly, because it consists of an infinite number of very different diagrams. But at this point, a rather systematic way of approximating the Green's function can be given: the one to approximate the self energy. This procedure is illustrated in Fig. 7: the self energy is approximated by one self-energy part, which for some reason is considered to be the most important one, and is being used in conjunction with the Dyson equation the calculate an approximation of the Green's function.

Let us look again at the bare Green's function

$$G^{(0)}(\boldsymbol{k},\omega)=\frac{1}{\omega-\xi_{\boldsymbol{k}}+i\delta_{\boldsymbol{k}}}$$

which is closely related to the excitation spectrum of the noninteracting system because it has poles at the unperturbed excitation energies. This property is shared by the full Green's function with respect to the interacting system:

$$G(\boldsymbol{k},\omega)=\frac{1}{\omega-\xi_{\boldsymbol{k}}-\Sigma(\boldsymbol{k},\omega)+i\delta_{\boldsymbol{k}}}\ . \tag{39}$$

The excitation energies of the perturbed system as obtained from (39) are

$$\begin{aligned} &\omega-\xi_{\boldsymbol{k}}-\Sigma(\boldsymbol{k},\omega)=0\\ \text{or}\quad &\omega=\xi_{\boldsymbol{k}}+\operatorname{Re}\Sigma(\boldsymbol{k},\omega)+i\operatorname{Im}\Sigma(\boldsymbol{k},\omega)\ . \end{aligned} \tag{40}$$

Note that due to the dependence of the self energy on the frequency, (40) is in general non-linear.

7.1 The self-energy of a phonon

The formalism presented so far is also applicable to calculating the phonon Green's function $D(\boldsymbol{q},\nu)$ in a perturbational approach from the bare phonon Green's function $D^{(0)}(\boldsymbol{q},\nu)$. The following Dyson equation defines the phonon self-energy $\Pi(\boldsymbol{q},\nu)$:

$$D(\boldsymbol{q},\nu)=D^{(0)}(\boldsymbol{q},\nu)+D^{(0)}(\boldsymbol{q},\nu)\Pi(\boldsymbol{q},\nu)D(\boldsymbol{q},\nu)\ . \tag{41}$$

As in the case of the electron self-energy, the phonon self-energy is given by all diagrams, which can be inserted between two phonon lines representing $D^{(0)}(\boldsymbol{q},\nu)$, but cannot be separated into independent parts by just cutting one phonon line.

An important contribution to the phonon self-energy is the decay of the phonon into an electron-hole pair with a subsequent recombination of the electron-hole pair and creation of a phonon. This process is depicted in Fig. 8, and, using the Feynman rules, can be translated into the expression

$$\Pi(\boldsymbol{q},\nu)=-2i|M_{\boldsymbol{q}}|^2\int\frac{d^3k\,d\omega}{(2\pi)^4}G^{(0)}(\boldsymbol{k}+\boldsymbol{q},\nu+\omega)G^{(0)}(\boldsymbol{k},\omega)\ .$$

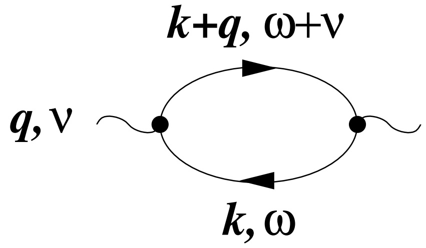

Figure 8: A irreducible contribution to the phonon self-energy.

As we will see later, this expression is very similar to the one for the longitudinal dielectric function.

We now evaluate the frequency integral in the expression above for a degenerate electron gas

$$\begin{aligned}\int \frac{d\omega}{2\pi} G^{(0)}(\boldsymbol{k}+\boldsymbol{q}, \nu+\omega) G^{(0)}(\boldsymbol{k}, \omega) \\ = \int \frac{d\omega}{2\pi} \frac{1}{\omega+\nu-\xi_{\boldsymbol{k}+\boldsymbol{q}}+i\delta_{\boldsymbol{k}+\boldsymbol{q}}} \frac{1}{\omega+\nu-\xi_{\boldsymbol{k}}+i\delta_{\boldsymbol{k}}} \ .\end{aligned}$$

We encounter four cases. The first is the case with $\xi_{\boldsymbol{k}+\boldsymbol{q}}$ above the Fermi surface and $\xi_{\boldsymbol{k}}$ below the Fermi surface, that is, the former corresponds to an electron and the latter to a hole. We close the integration contour in the upper frequency half plane and take the residue of the pole at $\omega = \xi_{\boldsymbol{k}} + i\delta$. The integral $\int d\omega$ equals to $2\pi i$ times the sum over all residues,

$$\int \frac{d\omega}{2\pi} \frac{1}{\omega+\nu-\xi_{\boldsymbol{k}+\boldsymbol{q}}+i\delta_{\boldsymbol{k}+\boldsymbol{q}}} \frac{1}{\omega+\nu-\xi_{\boldsymbol{k}}+i\delta_{\boldsymbol{k}}} = \frac{i}{\nu-(\xi_{\boldsymbol{k}+\boldsymbol{q}}-\xi_{\boldsymbol{k}})+i\delta} \ .$$

The second case deals with $\xi_{\boldsymbol{k}+\boldsymbol{q}}$ below the Fermi surface and $\xi_{\boldsymbol{k}}$ above the Fermi surface and results in the complex conjugate of the expression above. In the last two cases, either both poles are in the upper half plane or both are in the lower half plane. The contour can be closed in the half plane which does not contain a pole and the integral vanishes. Therefore, there are only contributions to the phonon self-energy from an electron and a hole, not from two electrons or two holes.

Adding all the contributions, from the different cases above, the resulting phonon self-energy becomes

$$\Pi(\boldsymbol{q}, \nu) = 2|M_{\boldsymbol{q}}|^2 \int \frac{d^3k}{(2\pi)^3} \left[\frac{1}{\nu-(\xi_{\boldsymbol{k}+\boldsymbol{q}}-\xi_{\boldsymbol{k}})+i\delta} + \text{c.c.} \right] \ .$$

This expression has poles at the energies $\xi_{\boldsymbol{k}+\boldsymbol{q}} - \xi_{\boldsymbol{k}}$ which are the excitation energies for pair excitations in which an electron from the state $\boldsymbol{k}$ is excited to the state $\boldsymbol{k} + \boldsymbol{q}$. Another very important property of the equation above is that its real part is even in frequency ν and its imaginary part is odd in frequency. This is a general rule for Green's functions and self-energies describing bosonic excitations. The excitation of fermion-pairs shares these properties.

8 Analytic properties of Green's function

In this section, we will take a closer look to the analytic properties of Green's functions and define retarded Green's functions.

The analytic properties of the Green's function are of central importance for the interpretation of many-particle effects. We will investigate these properties for the Green's function $G(\boldsymbol{k}, \omega)$ in frequency space. We recall that $G(\boldsymbol{k}, t)$ is defined only for real times although the Fourier transform defines $G(\boldsymbol{k}, \omega)$ in the whole complex frequency plane.

8.1 The spectral functions

The analytic properties of $G(\boldsymbol{k}, \omega)$ are brought clearly to light by introducing the *Lehmann representation*. We start with the definition of the Green's function (9) (the state $|\mathrm{GS}\rangle$ is the exact ground state of the system an we denote by N its particle number) and treat the case $t > t'$. By inserting the complete sum $\sum_n |n\rangle\langle n| = 1$ of eigenstates of H between the c-operators and using E_0 and E_n to denote the eigenenergies of the exact ground state $|\mathrm{GS}\rangle$ and the states $|n\rangle$, respectively, the expression

$$G(\boldsymbol{k}, t - t') = -i \sum_n \left|\langle n|c^+_{\boldsymbol{k}}|\mathrm{GS}\rangle\right|^2 e^{-i(E_n - E_0)(t-t')}$$

can be derived. The states $\langle n|$ must contain $N + 1$ particles. Therefore, the energy E_n is the energy of an eigenstate of the $(N + 1)$-particle system. If we denote by ω_n the energy difference between E_n and the ground state energy E_0 of the $(N + 1)$-particle system, and take into consideration that the difference of the ground state energies for the $(N + 1)$-particle and the N-particle systems, respectively, equals the chemical potential μ, the relation $E_n - E_0 = \omega_n + \mu$ holds. We consider the case for $t < t'$ and obtain an expression similar to the one above. Performing a Fourier transformation then yields the expression

$$\begin{aligned} G(\boldsymbol{k},\omega) = & -i\sum_n \left|\langle n|c_{\boldsymbol{k}}^{+}|\mathrm{GS}\rangle\right|^2 \frac{i}{\omega-\omega_n-\mu+i\delta} \\ & +i\sum_n \left|\langle \mathrm{GS}|c_{\boldsymbol{k}}^{+}|n\rangle\right|^2 \frac{-i}{\omega+\omega_n-\mu-i\delta}\ . \end{aligned}$$

We further simplify this expression by introducing the *spectral functions*

$$\begin{aligned} A(\boldsymbol{k},\omega') &= \sum_n \left|\langle n|c_{\boldsymbol{k}}^{+}|\mathrm{GS}\rangle\right|^2 \delta(\omega'-\omega_n) \\ B(\boldsymbol{k},\omega') &= \sum_n \left|\langle \mathrm{GS}|c_{\boldsymbol{k}}^{+}|n\rangle\right|^2 \delta(\omega'-\omega_n) \end{aligned}$$

which vanish for negative frequencies ω', because ω_n is non-negative. These functions have a useful physical interpretation. The expression $A(\boldsymbol{k},\omega)\,d\omega'$ $[B(\boldsymbol{k},\omega)\,d\omega']$ gives the probability that an electron [hole] with momentum $\boldsymbol{k}$ has an energy (measured from the Fermi energy) in the interval from ω' to $\omega'+d\omega'$. Consequently, the sum rule

$$\int_0^\infty A(\boldsymbol{k},\omega')\,d\omega' = 1-n_{\boldsymbol{k}} \qquad \left[\int_0^\infty B(\boldsymbol{k},\omega')\,d\omega' = n_{\boldsymbol{k}}\right]$$

expresses the fact that the electron [hole] with quasimomentum $\boldsymbol{k}$ has a positive energy (we use $n_{\boldsymbol{k}} = \Theta(|\boldsymbol{k}|-k_F)$). Note also the sum rule $\int(A+B)\,d\omega' = 1$.

Using the spectral functions, the Green's function can be written in the form

$$G(\boldsymbol{k},\omega) = \int_0^\infty d\omega' \left[\frac{A(\boldsymbol{k},\omega')}{\omega-\omega'-\mu+i\delta} + \frac{B(\boldsymbol{k},\omega')}{\omega+\omega'-\mu-i\delta}\right]$$

called the Lehmann representation. Taking the real and imaginary part, respectively, of this equation, it is easy to prove the relations

$$\begin{aligned} \operatorname{Im} G(\boldsymbol{k},\omega) &= \begin{cases} -\pi A(\boldsymbol{k},\omega-\mu) & \text{for } \omega>\mu \\ \pi B(\boldsymbol{k},\mu-\omega) & \text{for } \omega<\mu \end{cases} \\ \operatorname{Re} G(\boldsymbol{k},\omega) &= \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\operatorname{Im} G(\boldsymbol{k},\omega')\,\operatorname{sign}(\omega'-\mu)}{\omega'-\omega}\,d\omega' \end{aligned}$$

connecting the imaginary part of the Green's function $G(\boldsymbol{k},\omega)$ to the spectral functions $A(\boldsymbol{k},\omega)$ and $B(\boldsymbol{k},\omega)$, and relating the imaginary part of the Green's function to its real part by an equation similar to a Kramers-Kronig relation.

For a degenerate (noninteracting) electron gas, the spectral functions become δ-functions, that is

$$A(\boldsymbol{k},\omega) = (1-n_{\boldsymbol{k}})\delta(\omega-\epsilon_{\boldsymbol{k}}) \qquad A(\boldsymbol{k},\omega) = n_{\boldsymbol{k}}\delta(\omega-\epsilon_{\boldsymbol{k}}) \ .$$

Putting this into the Lehmann representation of the Green's function, Eq. (20) is easily recovered.

8.2 The retarded Green's functions

When calculating measurable quantities, as for instance the density of states, or the conductivity, or lifetime broadenings, it is convenient to utilize the retarded Green's functions. On the other hand, the retarded Green's function cannot be calculated directly, there is no diagrammatic expansion for retarded Green's functions. But the retarded Green's function is related in a simple way to the time-ordered Green's function used so far. Hence, the usual approach in calculating measurable quantities is to first determine the time-ordered Green's function by diagram techniques. Then the relation given below is used to find the retarded Green's function. The *retarded Green's function* $G_{\mathrm{R}}(\boldsymbol{k},t-t')$ is defined in the Heisenberg representation by

$$G_{\mathrm{R}}(\boldsymbol{k},t-t') = -i\Theta(t-t')\langle\mathrm{GS}|[c_{H,\boldsymbol{k}}(t),c^{+}_{H,\boldsymbol{k}}(t')]|\mathrm{GS}\rangle \tag{42}$$

with the commutator $[A,B]$. Because of the theta function $\Theta(t-t')$ the ω-t Fouriertransform of (42) only has poles in the lower half frequency plane. It is now easy to see that the relation between the time-ordered and the retarded Green's function is

$$\begin{aligned}\operatorname{Im} G_{\mathrm{R}}(\boldsymbol{k},\omega) &= \operatorname{Im} G(\boldsymbol{k},\omega)\cdot\operatorname{sign}(\omega-\mu)\\ \operatorname{Re} G_{\mathrm{R}}(\boldsymbol{k},\omega) &= \operatorname{Re} G(\boldsymbol{k},\omega)\end{aligned}$$

Due to the fact that the retarded Green's function is analytical in the upper frequency half plane, the following Kramers-Kronig relations hold:

$$\begin{aligned}\operatorname{Re} G_{\mathrm{R}}(\boldsymbol{k},\omega) &= \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\operatorname{Im} G_{\mathrm{R}}(\boldsymbol{k},\omega')}{\omega'-\omega}\\ \operatorname{Im} G_{\mathrm{R}}(\boldsymbol{k},\omega) &= -\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\operatorname{Re} G_{\mathrm{R}}(\boldsymbol{k},\omega')}{\omega'-\omega} \ .\end{aligned} \tag{43}$$

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